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ISSUES IN NUMERICAL SIMULATION OF FIRE SUPPRESSION

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ABSTRACT

This paper outlines general physical and computational issues associated with performing numerical simulation of fire suppression. Fire suppression encompasses a broad range of chemistry and physics over a large range of time and length scales. The authors discuss the dominant physical/ chemical processes important to fire suppression that must be captured by a fire suppression model to be of engineering usefulness. First-principles solutions are not possible due to computational limitations, even with the new generation of tera-flop computers. A basic strategy combining computational fluid dynamics (CFD) simulation techniques with subgrid model approximations for processes that have length scales unresolvable by gridding is presented.

INTRODUCTION

The purpose of this paper is to identify phenomenological and computational issues that drive requirements for the development of a fire suppression simulation capability. The ban on the production of halon by the Montreal Protocol, because of its ozone-depletion potential (ODP), has prompted significant research into finding a chemical replacement for Halon 1301. However, as the search for a 'drop-in' chemical replacement with the effectiveness of Halon 1301 continues, it is prudent to look to other areas of suppression-system performance for improvements.

In particular, it is of interest to look at improvements that can be achieved via control of transport phenomena (e.g., turbulent mixing) in addition to suppressant chemistry. For example, for a given chemical suppressant, increased system performance can be achieved through improving the uniformity of distribution of suppressant and increasing the turbulence levels in the flame as the suppressant arrives. The best overall performance can be achieved if there are no regions of excess suppressant within a volume at the time the suppressant concentration level exceeds that required to extinguish the fire. Regions of high concentrations represent wasted suppressant. Further, increasing the suppressant delivery velocity will increase the turbulence levels that will increase both the suppressant mixing rate and the strain on the flame and, thus, make a fixed amount of suppressant more effective.

A numerical simulation tool based on solution of transport equations (first-principles conservation equations) can be a vital aid in understanding suppression system performance if such a tool can incorporate the necessary phenomenology including the chemical performance of suppressants with sufficient fidelity to be relevant. As a first step in developing such a tool, it is necessary to identify the key phenomena, understand computer limitations, and investigate mathematical modeling strategies. These issues are the subjects of this paper.

A review of research on fire suppression is not intended, and in any case, would be impossible to provide within a reasonable space. The scope of the current study is also limited to gas phase suppressants against hydrocarbon flames that may be found in military platforms. In general, the next generation of suppressants may be gaseous, liquid, or solid particulate. In many cases, the actual suppressant effect of solids or liquids occurs in the gas phase, so that the current study may be viewed as a subset of the more general picture. Smoldering combustion is not considered.

Fire extinguishment strategies have a distinctly different goal than fire prevention or mitigation strategies. Fire extinguishment strategies work by eliminating exothermic chemical reactions. Prevention strategies eliminate the conditions that will lead to exothermic chemical reactions. Mitigation strategies accept the existence of exothermic reactions but seek to minimize damaging heat transfer (including suppressing but not extinguishing the fire). The authors' interest is primarily extinguishment, which is the limiting case of complete suppression. For the purposes of this research, fire extinguishment can be thought of as flame extinction throughout a compartment(s). Flame extinction is a very local, ultimately molecular, phenomenon while the compartments of interest to this study have length scales on the order of meters.

TIME AND LENGTH SCALES

Fire suppression involves a multitude of phenomena from convection of suppressant by turbulent flow, to strain modified-diffusion of suppressant into flame zones, to thermal and chemical interactions at the molecular level between the suppressant and fuel/air reaction species. It is important to recognize the length and time scales for suppression phenomena have very large ranges (Figure 1).

The smallest length scales of interest are the molecular collisional scales defined by the mean free path of the molecules, which are about 10^{-7} to 10^{-6} m, depending on the temperature at ambient pressure. The largest length scales are defined by the application under consideration, typically a compartment length-scale on the order of meters. The smallest time scales of interest are the molecular collisional times defined by the collision frequency of molecules, which is on the order of 10^{-10} sec depending on the temperature at ambient pressure. The largest time-scales are defined by the need to prevent thermally induced damage of aluminum, composite, or steel weapon platform materials by conduction heat-transfer time-scales, typically on the order of seconds to 10s of seconds. Therefore, representation of some 7 orders of magnitude in length scale and some 10 to 11 orders of magnitude in time scale are required to capture all the processes in fire suppression from molecular chemistry to the systems level.

The time and length scales shown in Figure 1 are determined from basic transport mechanisms. These mechanisms are shown in Figure 2. The two basic transport processes are random walk (diffusion) and mean directional flow (convection). These two processes result in three distinct regimes for information transfer with the random walk processes split between continuum and non-continuum length scales. Detailed information about these processes can be found in textbooks [1,2,3] and will only be described briefly below. Figure 2 is based on order of magnitude estimates at 1 atmosphere pressure.

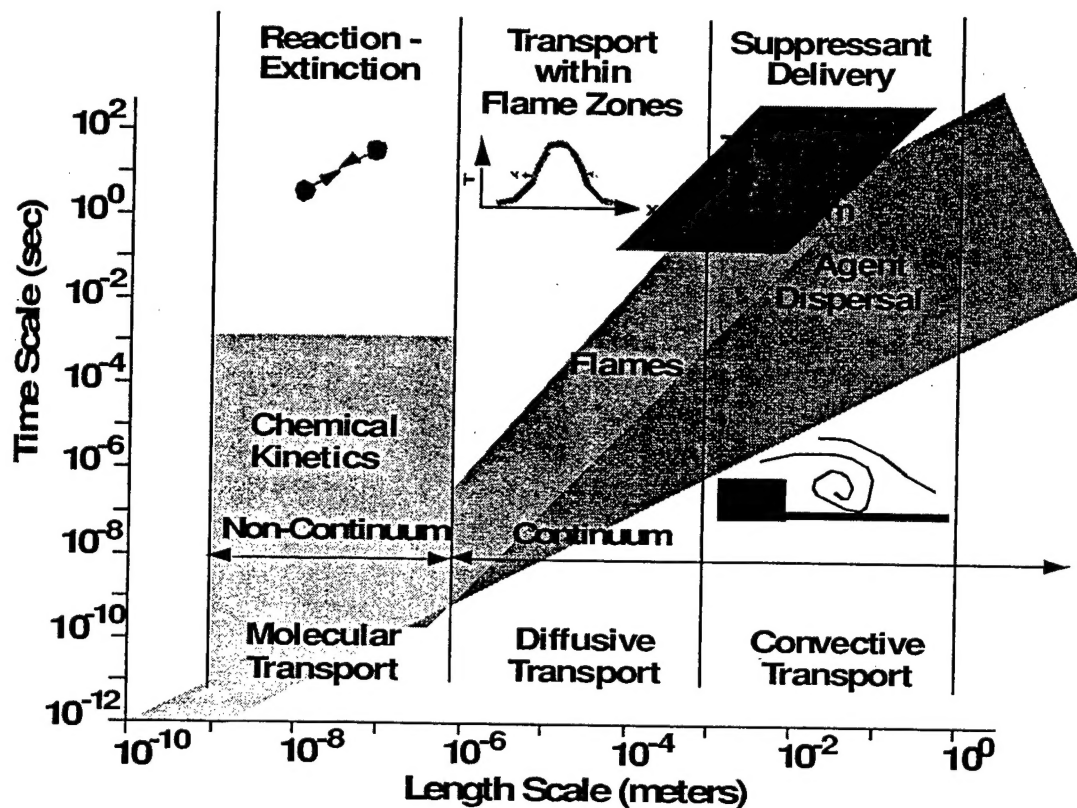


Figure 1. Fire and suppression time and length scales.

Information transfer is very fast over intermolecular distances (10^{-9} to 10^{-6} m) because molecular velocities are of order 500 m/sec at ambient conditions. At intermolecular distances, the characteristic time scale (τ in Figure 2) for information transfer is linearly dependent on the molecular velocity. While the molecular velocities are high, they are not directional but random.

Random walk processes are inefficient at transporting information in a given direction. The time scale for information transfer from a random walk process is proportional to the square of the distance over continuum length scales (above 10^{-6} m). Diffusion is the term applied to random walk processes at continuum length scales. Species, momentum, and energy transport all occur due to random walk processes that are described at a continuum level by their statistical properties, i.e., species diffusivity, viscosity, and thermal diffusivity, respectively.

Therefore, as shown in Figure 2, information takes much longer to transfer than one would expect given the high molecular velocity for length scales above roughly 10^{-6} m (temperature and pressure dependent) where sufficient molecules exist for continuum. From this length scale range to roughly 10^{-3} m (bulk velocity dependent), diffusion dominates the information transfer. At these length scales, it is the fastest information transfer process due to the high molecular velocities compared to the mean flow (convection) velocity. However, as distances become

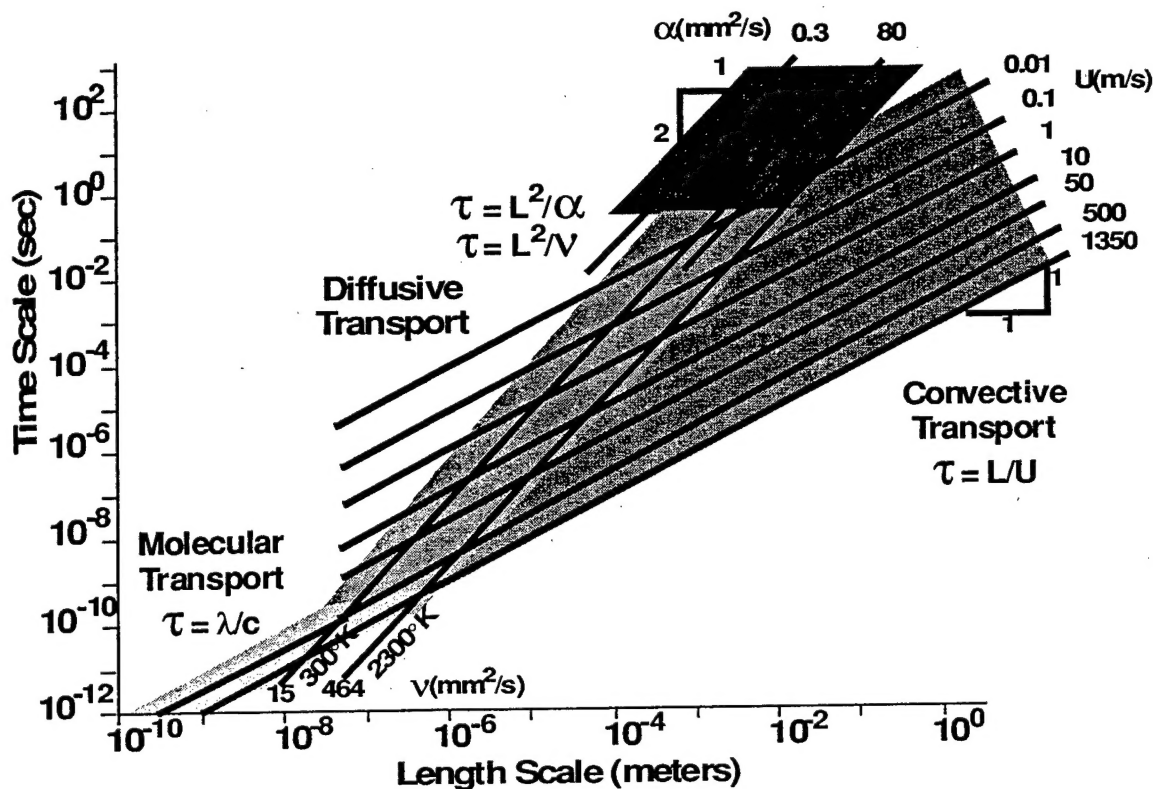


Figure 2. Transport process time and length scales.

greater, convection processes become faster at information transfer than random diffusional processes and begin to dominate information transfer. Depending on the characteristic velocity and diffusional characteristics, information is transferred faster by convection at length scales above the millimeter to centimeter level than by diffusion.

FIRE AND SUPPRESSION PHENOMENOLOGY

In this section, the authors will discuss the phenomena that need to be captured to produce a fire suppression model with engineering usefulness. The fundamental transport processes in Figure 2 determine the length scales and time scales for physical and chemical processes. Thus, a description of the phenomena important to suppression will be by process (or equivalently length scale over which that process is dominant).

At the smallest scales, molecular chemistry is dominant. Ultimately, local flame extinction will occur when the last molecular collision capable of sustaining the composition or temperature to sustain a flame is prevented. These collisional processes are represented at a continuum level by Arrhenius type reaction rates. The most important variables for these rates are species concentrations and temperature. These rate equations only apply over length scales in which the temperature and species are uniform. Diffusional processes result in gradients in the hundred micrometer

to millimeter scale in flames, limiting the length scale for which a given temperature and species concentration apply.

Three important features must be captured by a fire suppression model in this length scale regime: dilution, thermal suppression, and chemical suppression. All suppressants result in dilution. Dilution is simply the displacement of fuel or air molecules by suppressant molecules that lower the overall concentrations of fuel and oxygen. If the suppressant has a low temperature relative to the reactions in the flame zone, then it can lower the reaction temperature and, thus, slow the reaction rates for all elementary reactions occurring within that region. The magnitude of the effect is dependent on the heat capacity and temperature of the suppressant. If the suppressant is chemically active, then it can interfere with elementary reaction steps, e.g., chain branching by radical scavenging. Finding a chemically active suppressant is the subject of numerous halon replacement chemical studies of recent years. The research is difficult for many reasons, including toxicity, ODP, global warming potential, etc. Another is the complexity of the chemical mechanisms involved [cf. 4,5]. The construction of these chemical mechanisms to their current state of completion has taken many man-decades of work and represents a significant achievement in the understanding of flame chemistry and fire suppression. Ultimately, the chemical reaction rates are very temperature sensitive. Whether by dilution, thermal, or chemical suppression, when the temperature of the flame zone falls below a critical temperature, flame extinction will occur.

At larger length scales, diffusion produces gradients in temperature and species concentration creating what is recognizable as a diffusion flame. The character of this flame is determined by three factors: (1) the molecular chemistry that leads to heat release (primary reaction zone), (2) a balance between diffusional processes transporting heat and product species away from the reaction zone (and into the surrounding fuel and air to produce radicals), and (3) convection processes that, at times, are assisting or retarding the diffusional transport.

As an example, Figure 3a shows a simplified representation of a flame that exists in a shear layer. A section of this flame that has a mean convective inflow is idealized in Figure 3b as an opposed flow diffusion flame. In this flame, the mean convective inflow is balanced by outflow (flame stretch) along the axis of the flame. Since inflow occurs from both the air and fuel side, the inflow velocity must go to zero at the centerline. Therefore, a velocity gradient is set up normal to the flame. Velocity gradients that do not introduce rotational flow, strain the flow. In other words, the convective inflow into a stagnation region produces a strain in the flow. Hence, the flame is often referred to as a strained laminar diffusion flame. Increasing the inflow velocity increases the strain; at a critical level, which is dependent on temperature and suppressant concentrations, the flame extinguishes [cf. 6,7].

The most important feature to capture in the diffusional regime for a fire suppression model is extinction by flame strain. Figure 3c shows cross-sectional schematics of flames with different levels of inflow velocity (flame strain). As the inflow velocity increases, the width of the diffusion flame decreases [8] and the increased flow rate results in an increase in flame surface area. As the flame thins, species have less time residing in the flame before they are convected away [9]. It is reasonable to assume that this decrease in residence time most strongly affects

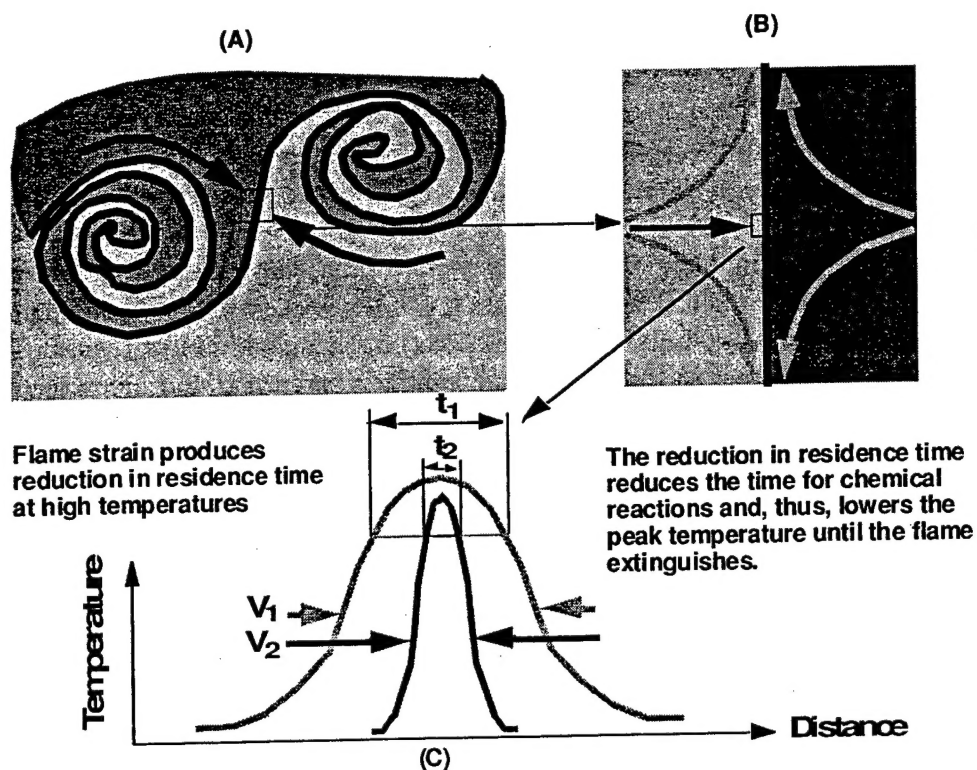


Figure 3. Schematic of a diffusion flame in a shear layer.

the slowest reactions [10,11]. These are the exothermic recombination reactions occurring at the center of the flame zone, which are producing the high temperatures that sustain the reaction rate. Hence, the temperature is lowered as these reactions have less time to complete. The lower temperature results in even longer completion times. Once a critical limit is reached, the reaction rates collapse leading to flame extinction.

This description is somewhat idealized for real fires since turbulent flow creates unsteady inflow-velocity, species, and temperature fluctuations on the flame, multidimensional diffusion effects resulting from flame curvature, and flame-flame interactions. These features may affect the quantitative requirements for flame extinction and are the subject of current combustion research. Also, in general, both diffusion and premixed flames can exist in a given region. However, premixed flame extinction can also be described in a similar manner [11].

The most important feature at convective length scales that must be captured in a fire suppression model is transport into and out of turbulent recirculation zones. Transport issues include momentum and suppressant mixing in turbulent flows. Military platforms typically have significant geometric complexity, which creates recirculation zones and turbulent eddies of all sizes from compartment scales down to diffusional scales.

Assuming an ignition source, the transport of fuel vapor and air must be captured sufficiently well to mark the flame zones that require extinction, particularly those that are hardest to

suppress. To the extent that buoyancy influences the overall flow during the suppression injection transient, then the heat release from the fire must also be captured. To the extent that the flow is dominated by momentum either from the pre-existing air flow or from the suppressant flow, capturing the heat release is second order.

Qualitatively speaking, the most difficult flames to extinguish are those that occur in regions of the flow that have a sustainable source of fuel and air, a reliable supply of high temperature products and/or radical species for ignition, low velocity gradients (strain), and little likelihood of having suppressant get to them. Previous studies have identified baffle- or step-stabilized spray or pool fires as having these characteristics and examined time scales for suppressant loading [cf. 12]. The transport into and out of recirculation zones is governed by pressure differences across the recirculation zone balanced by the pressure losses due to form drag and skin friction. This momentum balance will determine the velocity in the recirculation zone and hence the time-rate-of-change of suppressant concentration within the recirculation zone.

COMPUTATIONAL LIMITATIONS

It is assumed that a numerical simulation capability will be used for evaluation of existing suppression system designs and new/retrofit designs. As a design tool, multiple simulations will be required to produce an answer to the potential improvement of a given design. Hence, an order of magnitude estimate of the amount of computer time required is equal to the number of simulations multiplied by the time per simulation. The time per simulation is proportional to the number of spatial integration points (nodes) multiplied by the number of temporal integration points (time steps). The number of nodes in a problem is also (effectively) limited by the memory size of the computer. For workstation level machines and high-end personal computers, a large problem for design purposes with the intent to run many simulations is on the order of 10^5 nodes for short transients (hundreds of time steps). At best, one can expect in the foreseeable future that multiprocessor workstations will be able to repeatedly simulate 10^6 nodes. Only massively parallel, high performance computers will have higher processing power, but even they are limited to perhaps 10^9 nodes for design problems in the foreseeable future.

Figure 1 shows that the length scale range of important physical processes covers at least 6 orders of magnitude (even with assumptions that continuum approximations hold). To get a basic estimate of how many orders of magnitude in length scale can be simulated with a given number of nodes, one can take the cube root of the number of nodes. Assuming uniformly spaced grid nodes, this gives the length-scale range of the numerical simulation. Hence, one can expect to simulate 1.5 to 2 orders of magnitude in resolvable length scales from 10^5 to 10^6 nodes. Stated another way, for a given size of computer with a given resolution, it would take a machine with 1000 times the existing capability (speed/memory) to obtain 1 order of magnitude increase in spatial resolution. Further, an additional factor of 10 to 100 in computer speed, in the convective or diffusive regimes, respectively, would be needed to capture the shorter time scales associated with the increased spatial resolution. Therefore, of order 10^4 to 10^5 improvements are needed for each decade of length scale resolved. Given that there are at least six decades in length scales of importance to the problem, clearly numerical integration of all length scales will not be possible in the foreseeable future.

MATHEMATICAL MODELING ISSUES

In general for the continuum regime, the governing conservation equations (i.e., mass, momentum, and energy) are expressed in differential form. To obtain useful solutions, the equations must be integrated. Over certain flow regimes (e.g., laminar or simple geometry) closed form solutions exist for these equations. However, for turbulent flows, no general solutions of the Navier-Stokes equations are currently available. Therefore, the equations must be integrated numerically in an approximate manner using discrete representations of the equations evaluated at the node points.

However, we have observed that the number of integration points needed to capture continuum to compartment length scales is beyond foreseeable computers. Therefore, ideally one would like general, closed form, integral "solutions" to the physical processes over part of the length scale regime and approximate numerical integration over the balance. For engineering purposes, the length scales from the largest down to the scale of the grid affordable (i.e., centimeters if the problem is order meters) are usually chosen for numerical integration. Thus, one would like general, closed form, integral "solutions" to the physical processes over the length range from 10^6 m to the centimeter level, about 4 orders of magnitude. Unfortunately, over this range, the mathematical description of the physical processes is still the reacting form of the Navier-Stokes equations for turbulent flows for which no closed-form solutions exist.

Therefore, one is left with the inevitable task of coming up with approximations of sufficient accuracy to the physics in this regime to yield engineering solutions for fire suppression. The term applied to the integral approximations required to represent physical processes below the numerically resolved solution is "subgrid model" or "submodel." The physics resolved by numerical integration is usually called the 'grid solution.' Given the choices made, Figure 4 shows the split between the grid solution and the subgrid models for the fire suppression problem in compartments on the order of 1 m.

Given the need to use engineering approximations for part of the length and time scale range, and differential equations for the balance, the differential conservation laws must be modified to reflect that part of the range contained in submodels. This process is called filtering. Integral filters are passed over the governing Navier-Stokes equations, resulting in filtered terms. Filtered terms that can only be expressed by the integral effect of the unresolved scales on the resolved scales must be modeled by subgrid models. Two types of filters are commonly used: Reynolds-Averaged-Navier-Stokes (RANS) [cf. 13], a temporal filter, and Large Eddy Simulation (LES) [cf. 14], a spatial filter. In general, the physical and chemical processes are continuous in time and space so that filtering in one has implicit assumptions in the other. RANS is the older of the techniques and has a much broader filter width. As a result, modeling is implied even in the grid-resolved solution up to the integral scale of turbulence in the problem.

The physics captured by the grid solution is different for each technique. In general, therefore, the subgrid models for each will be different, since they need to capture the balance of the physical processes not captured by the filtered equations. However, for processes that have length and time scale spectra completely contained beneath the filter width of either technique, it is anticipated that there is little difference which filtering is chosen. For this reason, it is hoped

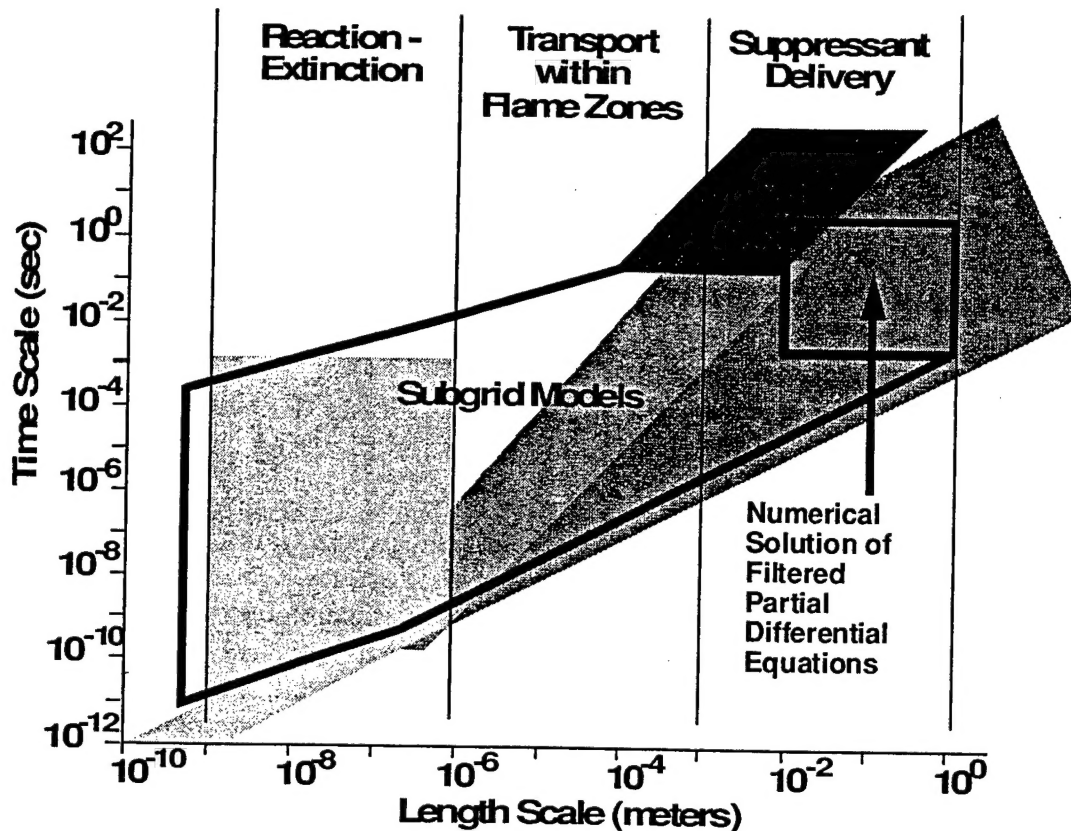


Figure 4. Physics representation by grid and subgrid models.

that a subgrid flame extinction model can be somewhat independent of the filtering technique used other than how convective information is passed to it from the turbulence momentum exchange process.

OUTLINE OF A SPECIFIC SUPPRESSION MODEL

Since there is no means of obtaining a first-principles solution due to computer hardware limitations, an unlimited number of approximate approaches may be taken. In this section, one approach that the authors are currently pursuing will be briefly outlined.

For a grid filter, RANS was chosen, because LES requirements for wall-bounded flows are currently the subject of significant discussion within the turbulence community [15,16]. For an overall suite of submodels for capturing fire, the one used by Magnussen's group was selected [17,18,19]. For a subgrid suppression model, we chose to expand on an approach used for flame extinction under high strain rate [20].

To lead order, the most important characteristic of a subgrid flame extinction model is that it turns off combustion in each cell when conditions dictate that suppression occurs and permits combustion to occur otherwise. Thus, the output can be a simple on/off switch with all the

chemistry and physics coupled to the decision of what state the switch should be in for combustion. This simple approximation permits a large degree of decoupling with the subgrid combustion model (of which there are many types) and, therefore, permits implementation into a variety of models. Its tie to the computational grid solution is through its on/off effect on the combustion model. In other words, if flame extinction occurs, then the filtered source terms in the conservation equations due to combustion are zeroed out. If not, they are unaltered.

The switch can be stated as a Damkohler number (Da) as follows:

$$Da_{critical} < \frac{t_{flow}}{t_{chemical}} \Rightarrow \text{Combustion Unaltered} \quad (1)$$

$$Da_{critical} \geq \frac{t_{flow}}{t_{chemical}} \Rightarrow \text{Combustion Terminated}$$

where t_{flow} and $t_{chemical}$, are characteristic time scales for flow and chemistry, respectively. The desired characteristic time scale for the flow is the residence time of a fluid particle in the flame zone. Since flames are a diffusive phenomenon and turbulence dissipation by viscous diffusion is also a diffusive phenomenon, it is reasonable to expect that the two time scales are proportional. Thus, the Kolmogorov time scale [21], based on the viscous dissipation, is used as an estimator of the local residence time in a flame zone. The time scale has a square root of viscous dissipation term, which is taken from the $k-\epsilon$ turbulence model. In this manner, turbulence on the grid is used to estimate the strain at the flame level.

The desired characteristic time scale for the chemistry is that occurring in a flame zone. Since the species and temperatures vary considerably across diffusive scales, a means of estimating the correct histories must be made. One method is to use one-dimensional calculations for strained laminar flames. To reduce the effort required, we use a perfectly stirred reactor (PSR) assumption, which is a simpler, but perhaps less accurate, approach requiring only a point calculation.

Therefore, the characteristic chemical time scale is taken to be the blowout time for the PSR. The blowout time is the minimum residence time below which reactions quench. Thus, it is an engineering approximation of the minimum chemical time necessary to prevent a flame from extinguishing. The blowout time varies dramatically as a function of pressure, temperature, and species composition (including suppressants). To capture the chemical effects, full chemistry is used [4,5]. This choice necessitates the need to pre-calculate these time scales as they are too computationally expensive to perform during the computer simulation.

If actual time scales were used instead of characteristic time scales using engineering approximations, then $Da_{critical}$ would have physical significance. As it is, $Da_{critical}$ reflects the lack of knowledge embedded in the engineering approximations. It must be determined empirically and is assumed to be a constant. Equation 1 is evaluated for every computational cell where combustion is occurring at every time step in a transient calculation. In practice, the residence time (t_{flow}) is calculated for each cell and is compared to the pre-calculated chemical time multiplied by $Da_{critical}$. If the residence time is too short, then flame extinction occurs within the computational cell, otherwise, the flame continues. Fire extinguishment occurs when local flame extinction occurs everywhere in the domain.

NEED FOR EXPERIMENTAL DATA SETS

The model contains one new constant, $Da_{critical}$, which must be specified by comparison to well controlled experimental data. Experiments are underway by Takahasi, Schmoll, and Belovich [22,23,24], which will be used to both calibrate the model and determine its range of validity around the calibration point. The constant will be set by comparing the calculated and measured suppressant concentration required to extinguish a flame stabilized behind a backward facing step with a significant imposed velocity over the step. Additional full-scale, in-situ data are then needed to confirm that the model has engineering usefulness.

CONCLUSIONS

The range of time and length scales involved in fire and its suppression are vast, spanning more than 6 orders of magnitude. Given existing and anticipated computational hardware limitations, first-principles calculations will not be achievable in the near future. Thus, a combination of grid resolvable models (derived from filtering first-principles conservation equations) and subgrid models (based on engineering principles such as dimensional reasoning) is required to adequately simulate fire suppression phenomena. The most important phenomena that must be captured in a fire suppression model can be characterized by transport processes. At convectively dominated length scales, fuel, air, and suppressant transport must be captured, principally in multiply interconnected recirculation zones created by the complex geometry in military platforms. At diffusionally dominated length scales, the effect of flame strain due to turbulence-induced velocity gradients on combustion chemistry must be captured. At scales within the reaction zone (small compared to diffusional gradients), the effect of suppressant dilution, heat capacity, and kinetic interaction (e.g., radical scavenging) on the heat releasing reactions must be captured. Since first-principles calculations cannot be made, experimental data for calibration, validation, and confirmation of the usefulness of the methodology in real, complex environments are required.

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